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Test Particle Monte-Carlo modelling of installations for NEG film pumping properties evaluation

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ABSTRACT

Two installations were built in the ASTeC vacuum science laboratory to investigate the pumping properties of non-evaporable getter (NEG) films. An important parameter to characterise the pumping properties is the film sticking probability (α). Test Particle Monte-Carlo (TPMC) models were used for accurate evaluation of NEG film sticking probability from pressure readings during gas injection. The results of these models were used for interpreting the results of measurements in different experimental configurations: planar, cup and tubular samples. It was shown that there is a difference between simple formulas used in vacuum technique and TPMC results which is significant for $\alpha > 0.1$ with planar samples, for $\alpha > 0.01$ with cup samples, and in the full range of α for tubular samples. It was also shown that the gauge positions are very important, the exact position of the gauge or RGA ionisation chamber should be used in the modelling.

1. Introduction

The NEG coating is a relatively new vacuum technology which allows optimisation and lowers the cost for the particle accelerator vacuum system [1–3]. The experimental installation for studying the pumping and capacity properties of the NEG coated films was designed and built in the ASTeC Vacuum Science group laboratory at Daresbury Laboratory (DL). The NEG coating pumping properties can be characterised with a sticking probability α for different gases as a function of the amount of sorbed gas per unit of its surface area A_{NEG}. The measurement system is based on the Dynamic Expansion Method with a gas injection system able to inject the gases present in the spectrum of a UHV system, such as H_2, CO, CO_2 and CH_4. There were a few different set-up configurations used in experiment to study flat, cup and tubular samples.

The only parameters measured in the experiment are inlet the gas flow and the pressure readings in the test vacuum chamber. In a vessel with a uniform molecular velocity distribution, pressure can be defined by a gas load Q and a pumping speed S as the following:

$$P = \frac{Q}{S}. \tag{1}$$

The pumping speed S, of surface A_{NEG}, with sticking probability α can be calculated with the formula:

$$S = \alpha A_{NEG}\frac{v}{4}; \tag{2}$$

where v is a mean molecular velocity for the injected gas. Therefore, the sticking probability can be calculated in this case as:

$$\alpha = \frac{4Q}{PA_{NEG}v} \tag{3}$$

As mentioned above the uniform molecular velocity distribution is required to apply Eqs. (1)–(3). However, these formulas are approximations when this condition fails, this may lead to a significant error, for example, when desorption and pumping surfaces are located in different parts of the vacuum system, especially when $\alpha \sim 1$.

To analyse the relationship between measured pressure(s) and the NEG coating sticking probability α the TPMC model was built and run for each configuration with the use of the MOLFLOW program written by R. Kersevan [4].

2. The Monte-Carlo modelling for data analysis

2.1. Test Particle Monte-Carlo (TPMC) model

The two installations built in the ASTeC vacuum science laboratory can be easily modified to allow measurements of either a flat, cup or tubular sample. Both test chambers are similar: dimensions

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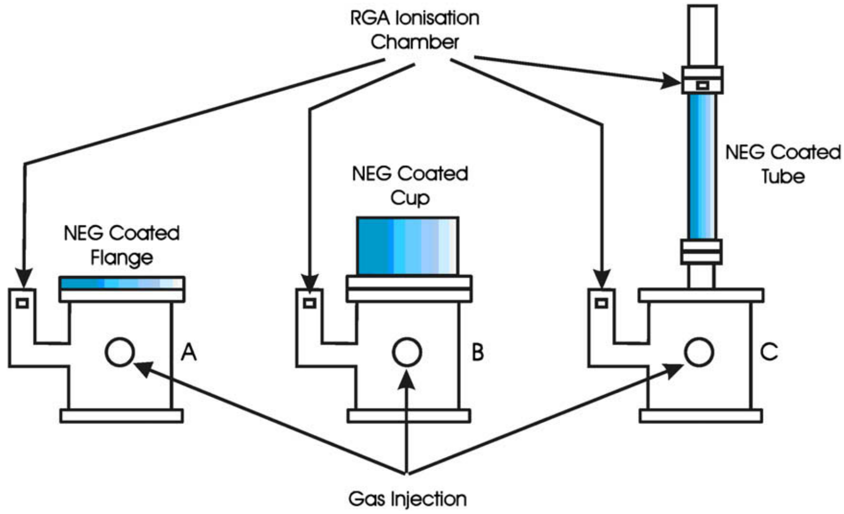

Fig. 1. Models for TPMC calculations: (a) planar sample, (b) cap sample and (c) tubular sample.

and locations of the RGA, extractor gauge and injection. Only the geometry of the NEG coated samples was different. Therefore, the TPMC models shown in Fig. 1 represented the three different NEG geometries. The TPMC model consists of a number of surfaces creating a closed volume, each surface (facet) has a number of assigned parameters; area, sticking probability, desorption (yes or no and if yes the angular distribution low, usually Maxwellian), reflectivity low (usually Maxwellian or mirror), and transparency. In our case, the only desorbing surface was the inlet surface of the injection line (see Fig. 1) and the only sorbing surface was the NEG sample surface. The model was run for discrete numbers of varied sticking probability α_i in the range $1\times10^{-3}\le\alpha\le1$ for the facet(s) representing the NEG coated sample. In each computational run i corresponding to α_i, the main result of the modelling is the number of hits $H_{i,j}$ counted at each facet j for the corresponding number of generated particles N_i. This value normalised to the number of generated particles N_i and the area of facet j, A_j, is called an impingement rate, which is defined as the following:

$$I_{i,j} = \frac{H_{i,j}}{A_j N_i}. \tag{4}$$

The average pressure P at each facet can be calculated for an injected gas flow Q as the following:

$$P_{i,j} = Q\frac{4I_{i,j}}{v}. \tag{5}$$

To investigate the pressure inside the RGA port as a function of sticking probability, a number of facets (which could be either opaque or transparent) were used in the model in the exact position and with the corresponding dimensions of the ionisation chamber of the RGA (see Fig. 1).

2.2. TPMC model results for flat and cup sample

The NEG coated surface was a flat sample, this is a 100-mm diameter disk with an area $A_f = 78.54\ \mathrm{cm}^2$ (see Fig. 1a). The cup sample was a 100-mm-ID and 100-mm long cylinder which is open on one side (see Fig. 1b). The side and bottom of the sample were NEG coated, the coated area was $A_c = 393.7\ \mathrm{cm}^2$, five times larger than the flat sample.

The results of the TPMC model can be used for calculating the pressure of any injected gas as a function of sticking probability for a given gas flow. An example is shown for CO injection in Fig. 2; a blue dotted line represents the flat sample, and a green dash-dot line represents a cup sample, both are shown for an injected gas flow of $Q = 10^{-7}$ mbar l/s These results when compared with ones calculated with formulas (1) and (2) (correspondingly, solid red and brown dash lines in Fig. 2) show that they match well for low sticking probability; but for larger sticking probabilities (i.e. $\alpha > 0.1$ for a flat sample and $\alpha > 0.01$ for a cup sample) the formulas (1) and (2) lead to errors. [For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.] Only the data obtained with TPMC modelling can be used to accurately determine the sticking probability of the NEG coating for various gases. However, to compute each point on this graph takes significant time, for example, for $N = 10^7$ test particles the model takes a few days for $\alpha = 10^{-3}$ to about a day for $\alpha = 1$. A fitting formula for these results obtained with the TPMC simulations can be used for practical calculations of the true sticking probability β from the pressure readings (see green dotted line in Fig. 3) in the experiments for a flat sample: [For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.]

$$\beta_f = \alpha\left(1 + 28\alpha + 0.13\alpha^2\right) \tag{6}$$

where α was calculated with formula (3).

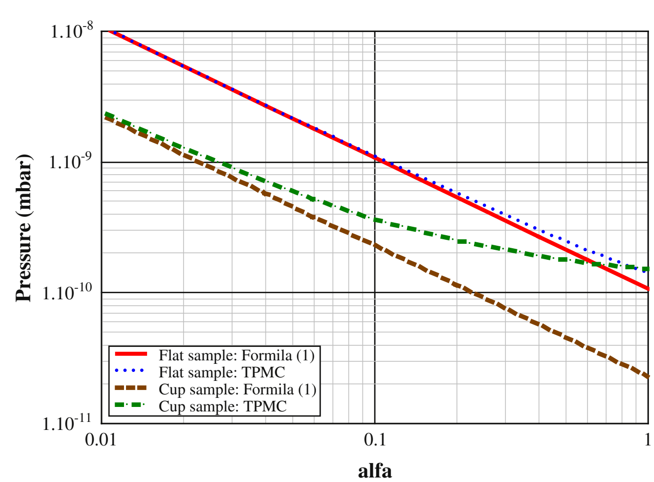

Fig. 2. A CO pressure at the gauge position as a function of sticking probability for NEG coated flat and cup samples corresponding to an injected flow of 10^{-7} mbar l/s.